



RIVER WATER QUALITY MODELLING: I. STATE OF THE ART

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ABSTRACT

River water quality models are used extensively in research as well as in the design and assessment of water quality management measures. The application of mathematical models for that purpose dates back to the initial studies of oxygen depletion due to organic waste pollution. Since then, models have been constantly refined and updated to meet new and emerging problems of surface water pollution, such as eutrophication, acute and chronic toxicity, etc. In order to handle the complex interactions caused by the increased influence of human activities in rivers it is today mandatory to couple river water quality models with models describing emissions from the drainage and sewerage system (such as the IAWQ Activated Sludge model No.1). In this paper-which is the first of a three-part series by the IAWQ Task Group on River Water Quality Modelling-the state of the art is summarized with the above aim in mind. Special attention is given here to the modelling of conversion processes but also the methods and tools to work with the models, i.e. parameter estimation, measurement campaign design, and simulation software, are discussed. © 1998 IAWQ Published by Elsevier Science Ltd. All rights reserved

KEYWORDS

Activated sludge model; eutrophication; oxygen household; rivers; software; water quality models.

INTRODUCTION

The IAWQ Task Group on River Water Quality Modelling was formed to create a scientific and technical base from which to formulate standardized, consistent river water quality models and guidelines for their implementation. This effort is intended to lead to the development of river water quality models that are compatible with the existing IAWQ Activated Sludge Models (ASM-1 and ASM-2, Henze *et al.*, 1987, 1995) and can be straightforwardly linked to them (or vice versa). Specifically, water quality constituents and model state variables characterizing O, N and P cycling are to be selected.

This paper is the first of a three-part series that analyses water quality modelling with the above aim in mind. It serves as a starting point and examines the existing state of the art in river water quality modelling. Part II (Shanahan *et al.*) looks at the limitations and problems of the current state of the art. Part III (Somlyódy *et al.*) builds on the first two papers to show possible directions for the future of the art with particular

attention to the specifications of standardized river water quality model state variables and process submodels that achieve the aims set out for the Task Group.

APPROACH TO RIVER WATER QUALITY MODELLING

River water quality models seek to describe the spatial and temporal changes of constituents of concern. Components or state variables have been gradually incorporated into models over the past seven decades following the evolution of water quality problems. Water quality models characterize among others oxygen household, nutrients and eutrophication, toxic materials, and so on. The complexity covers a broad range from the simple Streeter-Phelps model (Streeter and Phelps, 1925) with two state variables to QUAL2E and similar tools describing comprehensively O, N and P cycling with about ten state variables (Brown and Barnwell, 1987), to ecosystem models that may consider suspended solids, several classes of algae, zooplankton, invertebrates, plants, and fish (Boling *et al.*, 1975; Wlosinski and Minshall, 1983). The model choice depends on many different factors such as the objectives of the analysis, as well as data and time availability. Among the objectives two broad categories are usually distinguished: understanding/research and management/practice. Stemming from our goals, the Task Group has limited its attention to only models handling the "traditional" constituents O, N, and P.

Water quality changes in rivers due to physical transport and exchange processes (such as advection and diffusion/dispersion, the description of which requires one way or another the application of a hydraulic model as an input) and biological, chemical, biochemical, and physical conversion processes. The above processes in the water phase are governed by a set of well-known extended transport equations (see e.g. Somlyódy and van Straten, 1986).

$$\frac{\partial \mathbf{c}}{\partial t} = -\mathbf{u} \frac{\partial \mathbf{c}}{\partial x} - \mathbf{v} \frac{\partial \mathbf{c}}{\partial y} - \mathbf{w} \frac{\partial \mathbf{c}}{\partial z} + \frac{\partial}{\partial x} \left(\epsilon_x \frac{\partial \mathbf{c}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\epsilon_y \frac{\partial \mathbf{c}}{\partial y} \right) + \frac{\partial}{\partial z} \left(\epsilon_z \frac{\partial \mathbf{c}}{\partial z} \right) + \mathbf{r}(\mathbf{c}, \mathbf{p}) \quad (1)$$

where \mathbf{c} - n -dimensional mass concentration vector for the n state variables; t - time; x , y , and z - spatial coordinates; u , v , and w - corresponding velocity components; ϵ_x , ϵ_y , and ϵ_z - turbulent diffusion coefficients for the directions x , y and z , resp.; \mathbf{r} - n -dimensional vector of rates of change of state variables due to biological, chemical, and other conversion processes as a function of concentrations, \mathbf{c} , and model parameters, \mathbf{p} (subject to calibration). To Eq. (1) a mass conservation equation for the sediment should be added. Interface terms (sediment-water and water-air) appear as boundary conditions which are completed by further boundary and initial conditions (in- and outflows, zero mass fluxes across solid boundaries etc.).

Equation (1) is a well-known partial differential equation (PDE) that can be solved-together with the sediment equation-either numerically (usually after averaging over the depth or the cross-sectional area which reduces the number of dimensions and leads to the introduction of the so-called dispersion coefficient), or by using a conceptual approach that assumes that the system consists of m interconnected (completely mixed and/or plug flow) tanks or segments which leads to $n \times m$ ordinary differential equations. In both cases, some of the boundary conditions enter the simplified governing equations as boundary conditions (basically as a part of the aggregated conversion sub-model).

Equation (1) offers not only the basic governing equation of water quality models, but it also specifies a useful framework and the main model elements. These are the following:

- The hydrodynamic model for deriving velocity components u , v , and w , and turbulent diffusion coefficients ϵ_x , ϵ_y , and ϵ_z ;
- The transport (or advection-diffusion) equation (describing the behavior of so-called conservative substances) and its solution;
- The conversion sub-model, $\mathbf{r}(\mathbf{c}, \mathbf{p})$. It has much less solid theoretical grounds than hydrodynamics and, thus, for its development an adequate combination of theoretical and empirical knowledge is needed;

- For the latter purpose, methodologies such as calibration, validation, identification, sensitivity, and uncertainty analyses are required (Beck, 1987) which aid model selection and testing;
- The model designed on the basis of the above steps and elements should be implemented on a computer which raises a number of software (and hardware) issues.

Subsequently, we discuss the state of the art of water quality models for the components as listed above. The analysis will be short; for more details the reader is referred among others to Thoman (1972), Orlob (1982), Crabtree (1986), Thomann and Mueller (1987), McCutcheon (1989), and Somlyódy and Varis (1992).

HYDRODYNAMICS AND HYDRAULICS

Flow of water in a river is described by the continuity and momentum equations. The latter is known as the Navier-Stokes or Reynolds equation. The actual form of a hydrodynamic model depends on assumptions made on characterizing turbulence. Methods vary from the use of eddy viscosity as known parameters to the application of the so-called $k-\epsilon$ theory (see Bedford *et al.*, 1988 or Rodi, 1993 for an overview of the state of the art of turbulence models). Complex models are available (see e.g. Abbott, 1979; Naot and Rodi, 1982) but for water quality purposes mostly the well-known, cross-sectionally integrated (1D) Saint Venant equations or approximations to these equations are used (see e.g. Mahmood and Yevjevich, 1975; Abbott, 1979).

Many different forms and approximations to the Saint Venant equations are known, depending upon whether the flow is steady or unsteady and which simplifications are made. Thus, for water quality studies often the equation of steady, gradually variable flow is employed (which may be further simplified to the so-called Manning equation as done in QUAL2E). Unsteady models include the kinematic, diffusive, and dynamic wave approaches, all based on the continuity and momentum equations. The difference stems from simplifications of the latter: dynamic wave models solve the full equation, diffusive ones exclude the acceleration terms, while kinematic ones also disregard the pressure gradient term that is essential for the description of backwater effects. (Routing methods used widely in hydrology usually correspond to the last approach, see Mahmood and Yevjevich, 1975).

The hydrodynamic equations are generally solved by efficient finite difference methods (see e.g. Mahmood and Yevjevich, 1975). For water quality issues the acceleration terms in the momentum equation rarely play a significant role and the typical time scales are amplified by conversion processes. For these reasons, the diffusive wave approach is often a satisfactory approximation.

TRANSPORT PROCESSES

As seen from Eq. (1), the transport of dissolved substances in rivers is governed by advection and turbulent diffusion. The initial mixing in the 'near field' zone may depend on momentum transport; this is a phenomenon that is important if the discharge flow is large (e.g. thermal pollution). The transport process is characterized by two mixing lengths, L_1 and L_2 . These are the distances of 'complete' mixing along the depth and over the entire cross-section, respectively. For shallow rivers L_1 is short and thus a depth integrated 2D form of Eq. (1) can be applied. As a result of the integration, the impact of shear or spatial non-uniformity in the advective velocity appear in a term assumed to be of Fickian type, and the 'lumped' parameters of diffusion thus obtained are called dispersion coefficients. Their value strongly depend on slope, morphology, roughness etc. and can be taken from empirical formulas (Fischer *et al.*, 1979) or from in situ tracer measurements.

For water quality studies of rivers which are long in comparison to L_2 and dominated by longitudinal and temporal changes, further integration is possible along the width which leads to the 1D advection-dispersion equation (see e.g. Fischer *et al.*, 1979; alternatively the dispersion effect can be approximately described by dividing the river cross section into an advective and a stagnant zone, see e.g. Reichert and Wanner, 1991 and references cited therein). In a vector form corresponding to Eq. (1) this 1D equation can be written as:

$$\frac{\partial(AC)}{\partial t} + \frac{\partial(QC)}{\partial x} = \frac{\partial}{\partial x} \left(AD_L \frac{\partial C}{\partial x} \right) + AR(C, P) \quad (2)$$

where A = cross-sectional area; Q = streamflow rate; D_L = longitudinal dispersion coefficient (see Fischer *et al.*, 1979); C = vector of cross-section averaged concentrations of various constituents; $R(C, P)$ = vector of rates of change of cross-section averaged concentrations due to conversion processes which are now a function of model parameters, P expressed in terms of C . It is stressed that due to integration, the R functions and P parameters differ from r and p , respectively. Initial and boundary conditions are also needed to solve Eq. (2). The water quality model described by the function R can be developed step-wise and independently of the description of hydraulics.

For steady problems, the dispersion term can be often neglected and the resulting ordinary differential equation (ODE) can be solved by introducing the travel time as an independent variable. Often another simplification is made: Eq. (2) is integrated for subsequent river stretches within which complete mixing is assumed. This procedure leads to a sequence of interlinked reactors (and the application of the 'reactor principle') for which the mass balance is expressed by the vector equation

$$\frac{\partial(VC^*)}{\partial t} = Q_i C_i - Q C^* + V R^*(C^*, P^*) \quad (3)$$

where C^* = concentration vector; C_i = inflow concentration; Q_i = inflow; Q = outflow; V = reactor or tank volume and $R^*(C^*, P^*)$ = conversion rate vector (stars denote that the interpretation of C , R , and P is again different than in the 1D case). If the number of reactors is m , the $n \times m$ ordinary differential equations should be solved. Selection of the size of tanks should be done such that the introduced implicit or numerical dispersion is roughly equal to that of the actual system (see e.g. Shanahan and Harleman, 1984). Such box models are frequently used (e.g. Beck and Finney, 1987; Rauch and Harremoes, 1996), particularly due to the easier formulation of methods of calibration, validation, etc. in comparison to PDE model structures.

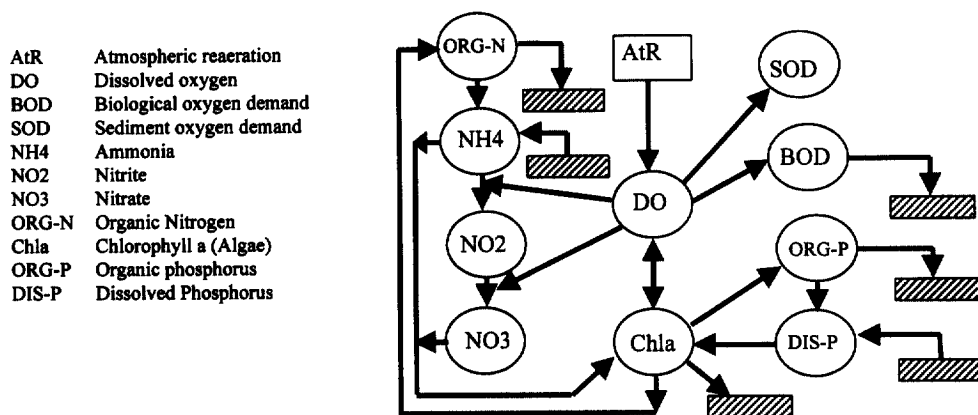


Figure 1. Schematic description of the water quality model QUAL2E (Brown and Barnwell, 1987).

CONVERSION PROCESSES

As noted, conversion processes describe changes in the constituent concentrations that are due to biological, chemical, biochemical, and physical processes. The historical development of O, N, and P models shows step-by-step extensions and increasing complexity as follows: (i) the starting point was the pioneer Streeter-Phelps model (Streeter and Phelps, 1925) describing the increase and following decrease of the oxygen

deficit downstream of a source of organic material, (ii) it was later extended by nitrogen processes (EPA's detailed model with nitrification was called QUAL1 [Orlob, 1982]); and (iii) finally phosphorus cycling and algae were added in creating the QUAL2 model family (Brown and Barnwell, 1987). Today, several versions of the state-of-the-art model QUAL2 are available (which also include refinements and extensions) depending on the purpose of the use (research, regulation etc.). Figure 1 shows schematically the processes included in this model.

The QUAL2E model includes degradation of organic material, growth and respiration of algae, nitrification (considering nitrite as an intermediate product), hydrolysis of organic nitrogen and phosphorus, reaeration, sedimentation of algae, organic phosphorus and organic nitrogen, sediment uptake of oxygen, and sediment release of nitrogen and phosphorus. All these processes consider the effect on oxygen, nitrogen and phosphorus cycles. The process formulations are given in Table 1 in matrix notation as introduced by Henze *et al.* (1987).

Table 1. Biochemical and physical processes of the river water quality model QUAL2E in matrix notation

Component	1	2	3	4	5	6	7	8	9	Process rate
Process	DO	BOD	ABM	ORG-N	NH ₄	NO ₂	NO ₃	ORG-P	DIS-P	[ML ⁻³ T ⁻¹]
1 Reaeration	1									K ₂ (DO _{sat} -DO)
2 Biodegradation	-1	-1								K ₁ ·BOD
3 BOD sedimentation		-1								K ₃ ·BOD
4 Sediment DO demand	-1									K ₄ /d
5 Photosynthesis	a ₃		1		-0.07·F _{NH4}		-0.07·(1-F _{NH4})		-0.01	μ _{max} ·ABM·f(L,N,P)
6 Respiration	-a ₄		-1	0.07				0.01		ρ·ABM
7 Algae sedimentation			-1							σ ₁ /d·ABM
8 Nitrogen Hydrolysis				-1	1					β ₃ ·ORG-N
9 Nitrification 1st step	-3.43				-1	1				β ₁ ·NH ₄ ·f(nitr)
10 Nitrification 2nd step	-1.14					-1	1			β ₂ ·NO ₂ ·f(nitr)
11 N sedimentation				-1						σ ₄ ·NH ₄
12 N sediment release					1					σ ₃ /d
13 P hydrolysis								-1	1	β ₄ ·ORG-P
14 P sedimentation								-1		σ ₅ ·ORG-P
15 P sediment release									1	σ ₂ /d

where DO = dissolved oxygen [ML⁻³]; DO_{sat} = DO saturation concentration [ML⁻³]; BOD = biochemical oxygen demand of organic material [ML⁻³]; ABM = algal biomass [ML⁻³]; ORG-N = organic nitrogen [ML⁻³]; NH₄ = ammonia-N [ML⁻³]; NO₂ = nitrite-N [ML⁻³]; NO₃ = nitrate-N [ML⁻³]; ORG-P = organic phosphorus [ML⁻³]; DIS-P = dissolved phosphorus [ML⁻³]; K₂ = reaeration coefficient [T⁻¹]; K₁ = deoxygenation coefficient [T⁻¹]; K₃ = BOD settling rate [T⁻¹]; K₄ = sediment oxygen demand rate [ML⁻²T⁻¹]; d = mean stream depth [L]; μ_{max} = maximum algal growth rate [T⁻¹]; ρ = algal respiration rate [T⁻¹]; σ₁ = algal settling rate [LT⁻¹]; σ₂ = benthos source rate for P [ML⁻²T⁻¹]; σ₃ = benthos source rate for N [ML⁻²T⁻¹]; σ₄ = N settling rate [T⁻¹]; σ₅ = P settling rate [T⁻¹]; β₁ = ammonia oxidation rate [T⁻¹]; β₂ = nitrite oxidation rate [T⁻¹]; β₃ = N hydrolysis rate [T⁻¹]; β₄ = P hydrolysis rate [T⁻¹]; a₃ = stoichiometric coefficient gO/gABM [-]; f(L,N,P) = algal growth limitation factor; f(nitr) = nitrification limitation factor; F_{NH4} = ammonia preference factor.

The process formulations of other river water quality models are similar, as is illustrated by the water quality module of the program MIKE11 (DHI, 1992) given in Table 2 in the same notation. In spite of this general similarity, there are some remarkable differences. The most important difference is the division of organic matter into dissolved, suspended, and sedimented fractions in MIKE11. This makes it possible to model the fraction of the sediment oxygen demand caused by settled organic matter mechanistically (process 5 of this model considers only additional oxygen demand e.g. by respiration of sessile algae) and to model the development of organic matter in the sediment (sedimentation, degradation and resuspension). The approach used in QUAL2E with constant fluxes of oxygen into and of nitrogen and phosphorus out of the sediment cannot account for changes in sediment quality and does not allow one to check if nutrient cycles are closed. A minor difference between QUAL2E and MIKE11 is the simplified treatment of nitrification in MIKE11 that ignores nitrite as an intermediate product. The description of the phosphorus cycle cannot be compared, because in MIKE11 phosphorus concentrations are calculated in another module which is not given in Table

2. Neither QUAL2E or MIKE11 makes an attempt to describe the populations of bacteria responsible for degradation and nitrification nor those of sessile algae.

Recent model developments include extensions of QUAL2E to the description of the silica cycle and of sediment (Cerco and Cole, 1995). Similar processes are also implemented in other modules of MIKE11 (DHI, 1992) and in the new river water quality program designed by the German Association for Water Pollution Control (ATV, 1996). The latter includes silica, several classes of algae, consumers, suspended solids, pH, metals and a description of the sediment in addition to the state variables used in QUAL2E. Higher trophic states are also included in older stream ecosystem models (Boling *et al.*, 1975; Wlosinski and Minshall, 1983).

Table 2. Biochemical and physical processes of the river water quality module of MIKE11 (there exist additional packages for phosphorous, eutrophication, heavy metals and sediment)

	Component	1	2	3	4	5	7	Process rate
	Process	DO	BODd	BODs	BODb	NH3	NO3	[ML ⁻³ T ⁻¹]
1	Reaeration	1						K2·(DO _{sat} -DO)
2a	BODd biodegradation	-1	-1					Kd3·BODd
2b	BODs biodegradation	-1		-1				Ks3·BODs
2c	BODb biodegradation	-1			-1			Kb3·BODb
3	BOD sedimentation			-1	+1			K5·BODs/d
4	BOD resuspension			1	-1			S1·BODb/d
5	Sediment DO demand	-1						B1
6	Nitrification	-Y1				-1	1	K4·NH3 ^{e4}
7	Denitrification						-1	K6·NO3 ^{e6}
8	Photosynthesis	1				-0.066		Pmax·cos[2π(τ/α)]
9	Respiration	-1				0.066		R

where BODd = dissolved BOD [ML⁻³]; BODs = suspended BOD [ML⁻³]; BODb = settled BOD [ML⁻³]; Kd3 = degradation rate constant for dissolved BOD [T⁻¹]; Ks3 = degradation rate constant for suspended BOD [T⁻¹]; Kb3 = degradation rate constant for settled BOD [T⁻¹]; K5 = sedimentation rate for suspended BOD [LT⁻¹]; d = mean river depth [L]; S1 = resuspension rate for sedimented BOD (zero, if the flow velocity or the concentration BODb are below critical values) [LT⁻¹]; B1 = constant value of sediment oxygen demand (in addition to biodegradation of BODb) [ML⁻³T⁻¹]; Y1 = yield factor for oxygen consumed by nitrification [-]; K4 = nitrification rate constant [T⁻¹ or M^{1/2}L^{-3/2}T⁻¹]; e4 = coefficient characterizing concentration dependence of nitrification (1 or 0.5) [-]; K6 = denitrification rate constant [T⁻¹ or M^{1/2}L^{-3/2}T⁻¹]; e6 = coefficient characterizing concentration dependence of denitrification (1 or 0.5) [-]; Pmax = maximum production at noon (zero during the night) [ML⁻³T⁻¹]; τ = actual time of the day related to noon [-]; α = actual relative day length [-]; R = respiration rate [ML⁻³T⁻¹]. See Table 1 for other variables.

In addition to using temperature dependent rates (temperature dependence was omitted in Tables 1 and 2 for reasons of clarity), most advanced water quality models including QUAL2E and MIKE11 contain submodels that calculate water temperature. These submodels use short and long wave solar and atmospheric radiation, evaporation and sensible heat fluxes, and long wave emission in order to calculate river water temperature from a heat balance.

MODEL IDENTIFICATION AND TESTING

Experiments and data collection are crucial for testing and selecting conversion sub-models but are often inadequate (see Shanahan *et al.*, submitted). Provided adequate data are collected, the values of model parameters must be assessed from the data. Typically one starts from the default values that are reported with the model description. For complex models frequently nothing more than fine tuning is applied. In many practical applications of water quality models heuristic approaches are followed to decide which parameters to adjust to obtain a 'good' fit, choosing parameter values manually rather than by automated numerical techniques. Automated methods, on the other hand, depend on the model structure (PDE, ODE, linear, non-linear), noise assumed, loss function defined (e.g. minimization of the sum of least square deviations), optimization method (batch or recursive estimation), number of variables and parameters, type of measurements, and so on (see among others Beck and van Straten, 1983; van Straten and Somlyódy, 1986; Beck, 1987).

For smaller models - if a white noise assumption holds and regular observations are available - the Kalman filter or the extended Kalman filter can be applied. For more complex or non-linear models, the HSY method offers attractive features (Young *et al.*, 1987) and accounts for the fact that in water quality studies generally irregular data are available. Further useful techniques of calibration, validation, uncertainty, and sensitivity analyses are discussed by Beck (1987).

Table 3. Important software products (after Ambrose *et al.*, 1996, with extensions)

	PROGRAM	1	2	3	4	5	6	7	8	9	10
Hydrodynamics	Extern. Input	Y	Y	N	N	Y	N	N	N	N	Y
	Simulated	N	Y	Y	Y	Y	Y	Y	Y	Y	Y
	Control structure	N	N	Y	Y	Y	Y	Y	Y	Y	Y
Transport	Advection	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
	Dispersion	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Sediment	Quality models	N	Y	Y	N	Y	Y	N	N		Y
Water quality	Temperature	Y	N	Y	Y	Y	Y	Y	open structure	open structure	N
	Bacteria	N	N	Y	Y	Y	Y	Y			N
	DO-BOD	Y	Y	Y	Y	Y	Y	Y			Y
	Nitrogen	Y	Y	Y	Y	Y	Y	Y			Y
	Phosphorus	Y	Y	Y	Y	Y	Y	Y			Y
	Silicon	N	N	Y	N	Y	Y	Y			N
	Phytoplankton	Y	Y	3	Y	Y	Y	Y			Y
	Zooplankton	N	N	Y	N	Y	Y	N			N
	Benthic algae	N	N	N	N	Y	Y	Y			N
Systems analysis	Parameter estimation	N								Y	Y
	Sensitivity/uncertainty analysis	Y								Y	Y

1 = QUAL2E (US EPA; Brown and Barnwell, 1987); 2 = WASP5 (US EPA; Ambrose *et al.* 1988); 3 = CE-QUAL-ICM (US Army Engineer Waterways Experiment Station; Cerco and Cole, 1995); 4 = HEC5Q (US Army Engineer Hydrologic Engineering Center, HEC 1986); 5 = MIKE11 (Danish Hydraulic Institute; DHI 1992); 6 = ATV Model (ATV, Germany; ATV, 1996); 7 = Salmon-Q (HR Wallingford, UK; Wallingford Software 1994); 8 = DUFLOW (University of Wageningen, The Netherlands, Aalderink *et al.*, 1995); 9 = AQUASIM (EAWAG, Switzerland; Reichert, 1994); 10 = DESERT (IIASA; Ivanov *et al.*, 1996).

SOFTWARE AND COMPUTER PROGRAMS

Other than the simplest approaches, all mathematical models for prediction of water quality in rivers require the use of a computer to be worked with. Due to the considerable effort needed to develop and implement a site-specific model, the use of existing computer programs is preferred whenever possible. The following classification only aims to give an overview of the most important computer programs and is by no means meant to be exhaustive. Relevant features for classification are the description of hydrodynamics and transport, model structure (important variables, processes and submodels), software structure (open/closed - meaning that the user can change the model structure), and systems analytic features supported by the program. Table 3 gives an overview of some important software products for river water quality modelling.

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